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14. ABSTRACT The discovery of graphene, made of an individual atomic-thick layer of carbon, could be considered as a defining point in the research and development of stable truly 2D material systems. This breakthrough has opened up the possibility of isolating and exploring the fascinating properties of atomic layers of other layered materials in the form of MeX <sub>2</sub> (where Me = transition metal such as Mo, W, Ti, Nb, etc. and X = S, Se, or Te), and hexagonal boron nitride (hBN), which upon reduction to single/few atomic layers, will offer functional flexibility, new physical, chemical properties and novel applications. Each of these material systems exhibit specific properties that					
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## Report Title

Final Report: Beyond Graphene: Advanced 2D Electronic and Optoelectronic Crystals and Devices for Next Generation Applications

### ABSTRACT

The discovery of graphene, made of an individual atomic-thick layer of carbon, could be considered as a defining point in the research and development of stable truly 2D material systems. This breakthrough has opened up the possibility of isolating and exploring the fascinating properties of atomic layers of other layered materials in the form of MeX<sub>2</sub> (where Me = transition metal such as Mo, W, Ti, Nb, etc. and X = S, Se, or Te), and hexagonal boron nitride (hBN), which upon reduction to single/few atomic layers, will offer functional flexibility, new physico-chemical properties and novel applications. Each of these material systems exhibit specific properties that complement the technological goals of many applications, including field effect transistors, photodetectors, chemical and biological sensors, and nano-electromechanical systems. However, there are multiple, well defined challenges to synthesis of electronic-grade layered materials, heterogeneous integration of these films, development of devices that utilize the unique properties of these materials.

Therefore, addressing approaches to model, synthesize, and integrate these materials will enable the R&D community to develop nanodevices on an industrial scale. This will not only enhance scientific and technological understanding, but also have a broad impact on today's DoD technologies. The goal of the workshop was to bring together the nation's top researcher scientists and engineers to discuss 2D atomic layers, and to generate interest within the academic, industrial, and military R&D community to catalyze a synergistic research effort in these novel electronic material systems, and to answer the challenges of this exciting field. The workshop will bring together a wide spectrum of program managers and researchers within the military R&D community, industry, and academia as a means to generate potential topics in "electronic grade" layered materials and nano-device.

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Number of Presentations: 0.00

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Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

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Peer-Reviewed Conference Proceeding publications (other than abstracts):

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Graduate Students

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### Names of Faculty Supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>	National Academy Member
Joshua Robinson	0.00	
<b>FTE Equivalent:</b>	<b>0.00</b>	
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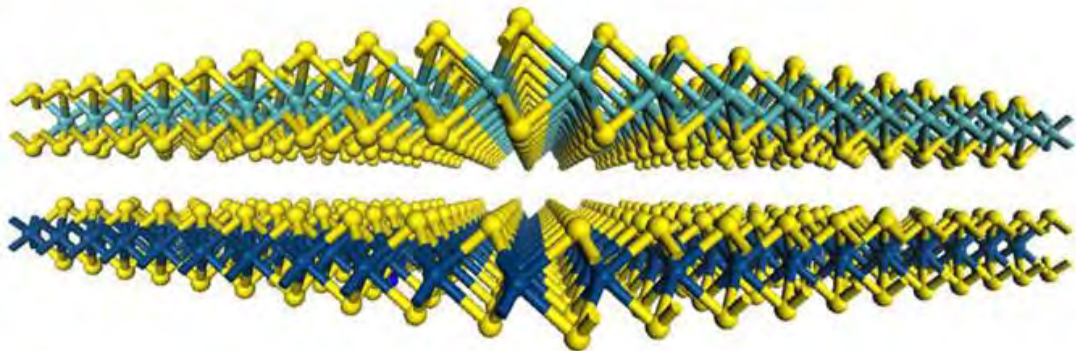
**Technology Transfer**

# **Workshop Final Report**

## **Beyond Graphene: Advanced 2D Electronic and Optoelectronic Crystals and Devices for Next Generation Applications**

**March 6-7, 2013**

**The Pennsylvania State University, University Park, PA**



***[http://www.mri.psu.edu/events/beyond\\_graphene/](http://www.mri.psu.edu/events/beyond_graphene/)***



## **Report Outline**

- I. Introduction
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- III. Programming Summary
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  2. Synthesis
  3. Theory of 2D Materials
  4. Properties of 2D Materials
  5. Devices and Application
- IV. Beyond Graphene Panel Discussion Digest: Now and Future
  1. Searching for certain Applications that can make 2D Materials Valuable
  2. Heterostructures of Beyond Graphene 2D Materials
  3. Approach of Optical Applications of 2D Materials
  4. Piezoelectric Feature of 2D Materials
- V. Beyond Graphene Workshop Survey: Improving for Next Year

## **Introduction**

The discovery of graphene, made of an individual atomic-thick layer of carbon, could be considered as a defining point in the research and development of stable truly 2D material systems. This breakthrough has opened up the possibility of isolating and exploring the fascinating properties of atomic layers of other layered materials in the form of  $\text{MeX}_2$  (where Me = transition metal such as Mo, W, Ti, Nb, etc. and X = S, Se, or Te), and hexagonal boron nitride (hBN), which upon reduction to single/few atomic layers, will offer functional flexibility, new physico-chemical properties and novel applications. Each of these material systems exhibit specific properties that complement the technological goals of many applications, including field effect transistors, photodetectors, chemical and biological sensors, and nano-electromechanical systems. However, there are multiple, well defined challenges to synthesis of electronic-grade layered materials, heterogeneous integration of these films, development of devices that utilize the unique properties of these materials. These challenges/opportunities include:

- No established methods of multi-scale modelling of these new materials systems
- Synthesis of large area metal dichalcogenide monolayers, capable of achieving carrier mobilities within 10x of mechanically exfoliated (non-scalable) methods.

**Two-Dimensional Electronic and Optoelectronic Materials: From Theory to Applications;** March 5-6, 2013; Penn State University; University Park, PA

( $\sigma_{e/h} > 100 \text{ cm}^2/\text{Vs}$ )

- Controlled-doping of pristine films for charge carrier modulation has not been demonstrated.
- Lack of established process/property/performance relationships easily accessible for rapid prediction of material performance via non-destructive means in an industrial setting.
- Heterogeneous assembly of dichalcogenide 2D atomic layers for band structure engineering has not been attempted.
- Transistor designs for high performance applications based on dichalcogenides does not exist.
- Benchmarking of dichalcogenide-based devices has not occurred.

Therefore, addressing approaches to model, synthesize, and integrate these materials will enable the R&D community to develop nanodevices on an industrial scale. This will not only enhance scientific and technological understanding, but also have a broad impact on today's DoD technologies. **The goal of the workshop was to bring together the nation's top researcher scientists and engineers to discuss 2D atomic layers, and to generate interest within the academic, industrial, and military R&D community to catalyze a synergistic research effort in these novel electronic material systems, and to answer the challenges of this exciting field.** The workshop will bring together a wide spectrum of program managers and researchers within the military R&D community, industry, and academia as a means to generate potential topics in "electronic grade" layered materials and nano-device.

## Workshop Schedule

Wednesday, March 06, 2013, HUB, Alumni Hall	
Time	Activity
7:30	Breakfast/Registration
8:40	Welcome: Joshua Robinson (PSU)
8:50	Penn State Research: Carlo Pantano (PSU)
9:10	Penn State Research Initiative in 2D Materials: Terrones (PSU)
9:30 - 10:30	Perspectives
9:30	Pani Varanasi (ARO)
9:30	Anupama Kaul (NSF)
10:00	Berry Jonker (Naval Research Lab)

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10:30	Coffee Break
10:45 - 12:15	Synthesis Rudresh Ghosh (University of Texas at Austin) Mauricio Terrones (PSU) Manish Chhowalla (Rutgers)
12:15	Lunch (on your own)
1:15 - 2:45	Theory Vivek Shenoy (UPenn) Boris Yakobson (Rice) Evan Reed (Stanford)
2:45	Coffee Break
3:00 - 4:00	Properties Humberto Gutierrez (Louisville) Pulickel Ajayan (Rice)
4:00 – 5:00	Panel Discussion: Perspectives on 2D Materials: Robinson (PSU)
5:00	Tour of Millennium Science Complex
6:00 - 7:00	Poster Reception: Hors d'oeuvres & Refreshments

Thursday, March 07, 2013, HUB Alumni Hall	
Time	Activity
7:30	Breakfast
8:30 - 10:30	Properties and Devices Adam Friedman(NRL) Jie Shan (Case Western) Michael Strano (MIT) Fengnian Xia (IBM)
10:30	Break
10:45 - 12:15	Devices and Applications Jeorg Appenzeller (Purdue) Debdeep Jena (ND) Sayeef Salahuddin (Berkeley)
12:15	Wrap-up
12:30	Adjourn

## **Programming Summary**

### **PART 1. Perspectives**

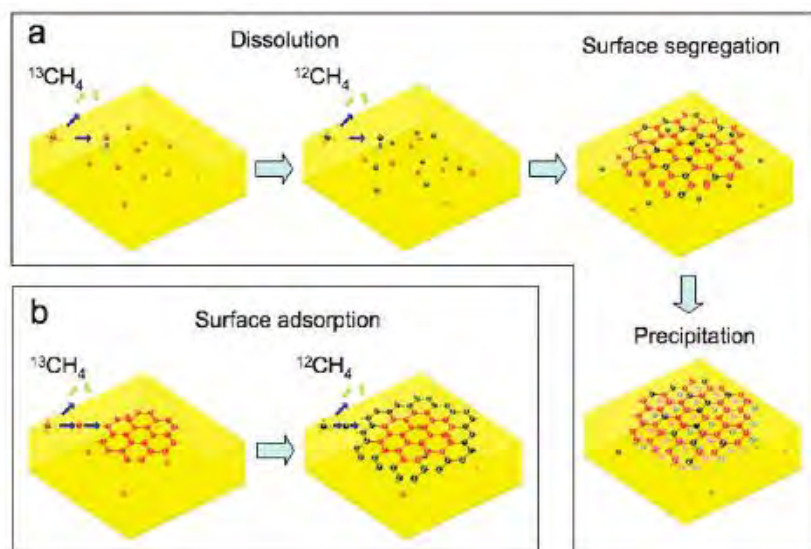
In this session, many perspectives and expectation on graphene and beyond graphene 2D layered materials were brought out and discussed. Dr. Varanasi talked about expectation from Army Research Office.. Army relevant research in 2D materials area is presently focusing on physical properties of materials and new technologies with revolutionary new capability or improvement of existing ability. Materials scientific division in ARO is working on defect sciences and engineering, and electronic, phonic, magnetic, thermal, thermal as well as the underlying physic properties of 2D materials. From the point of view from ARO, 2D materials have great opportunities to be applied to flexible electronic in army. In order to approach this, 2D materials still need more development, not only materials processing and characterization, but also theoretical modeling for fundamental understanding, process engineering corresponding with novel device concepts.

On the other hand, Dr. Jonker from Naval Research Lab provided an overview on graphene-like 2D layered systems including transitional metal dichalcogenides, oxides and nitrides which have an exciting spectrum of electronic, optical, thermal and mechanical properties. Dr. Jonker introduced that graphene is great for magnetic tunneling junction because of its discrete thickness, chemically inert, impervious diffusion, thermally robust and excellent spin filter. 2D materials also have magnetic tunneling junction due to their (1) high degree spin filtering ability; (2) spin injection/detection that could solve conductivity mismatch; (3) geometrically consistent window for 22nm mode. Dr. Jonker also gave a broad overview on 2D materials on photonic and magnetic devices (EPMD) and communication cyber systems (ECCS) which proves that this is an important class of materials.

### **PART 2. Synthesis**

Starting from graphene synthesis, this session brought us the latest results on graphene and graphene-like 2D materials synthesis. Post-doctoral scholar R. Ghosh from Dr. Ruoff's group in University of Texas, Austin presented a summary of their recent progress on graphene and hBN synthesis. Various substrates were tested for chemical vapor deposition (CVD) process on graphene growth, and copper and nickel were the best choices for extensive graphene growth due to low cost and carbon solubility at 1000C. Graphene growth process was determined to be a surface catalyzed process rather than precipitation mechanism by studying the relation between time and film thickness with coverage. The large area roll-to-roll (R2R) production of graphene films brought out by Dr. Ruoff's group could be the biggest

improvement for future application.



**Figure 1.** Schematic diagrams of the possible distribution of C isotopes in graphene films based on different growth mechanisms for sequential input of C isotopes. (a) Graphene with randomly mixed isotopes such as might occur from surface segregation and/or precipitation. (b) Graphene with separated isotopes such as might occur by surface adsorption.

*X. Li, W. Cai, L. Colombo and R. S. Ruoff, Nano Letters, vol.9, No. 12, 4268-4272, 2009*

On beyond graphene 2D materials, Dr. Ruoff's group also reported their recent synthesis on hexagonal Boron Nitride (h-BN) thin films. Similar to their graphene synthesis process, h-BN was brought by a similar CVD route, but with  $\text{B}_2\text{H}_6$  precursor and  $\text{NH}_3$  as starting materials on nickel substrate. Raman spectroscopy with peak position around  $1365\text{cm}^{-1}$  was determined for h-BN  $\text{E}_{2g}$  fingerprint, along with HR-TEM images showing the layered h-BN, and UV-Vis spectroscopy result showing 5.75eV band gap, Dr. Ruoff's group has shown a non-surface limited growth process for h-BN material. H-BN growth mechanism was studied by ALD like approach, using  $\text{B}_2\text{H}_6$  with  $\text{NH}_3$  gas reacted at  $1025^\circ\text{C}$  which differ from previous used  $\text{BH}_3$  precursor, surface diffusion and precursor decomposition models were examined for BN forming reaction. XPS results on relation of B-O, B-Ni peaks and  $\text{NH}_3$  gas feed have proved that Boron precursor would first form a B-Ni phase then improves h-BN thin film formation due to similar low solubility for B and N on Cu and Ni substrate. Their current work would be to obtain large domains of single or few layer h-BN on Ni that can be used for multiple device purposes.

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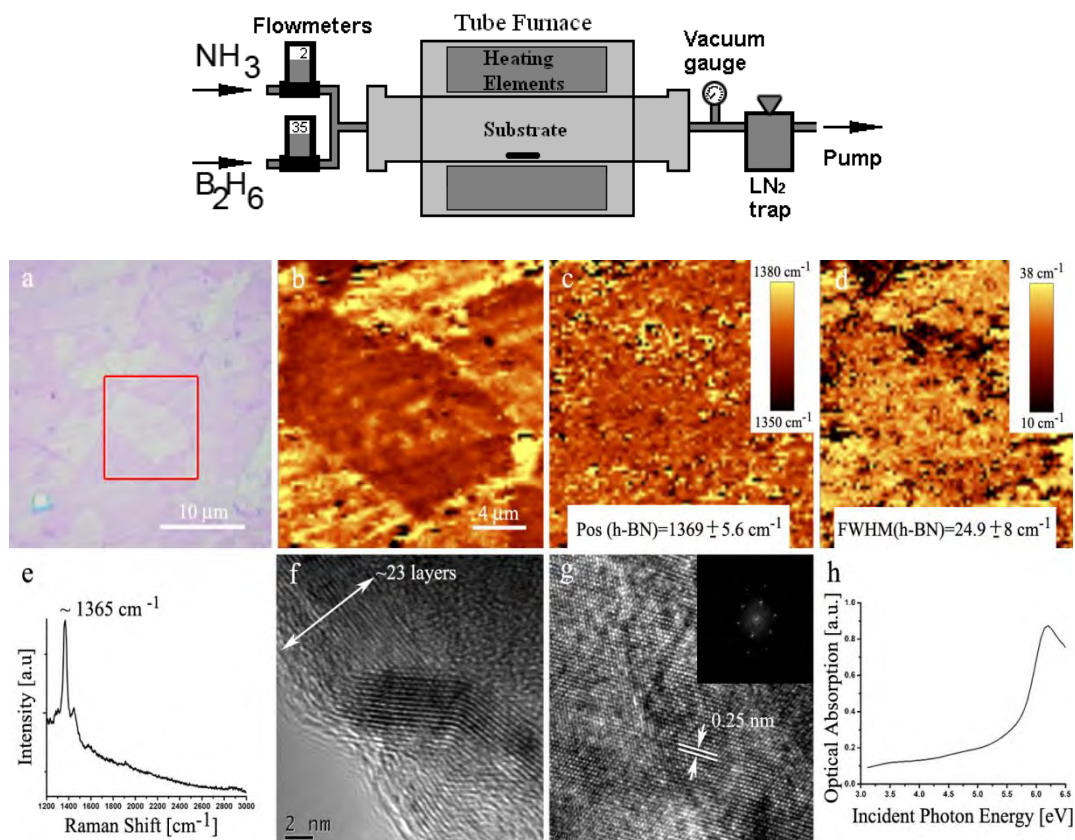


Fig. 2 Schematic plot and characterization for layered h-BN growth.

A. Ismach et al., ACS Nano, vol. 6, No. 7, 6378-6385, 2012

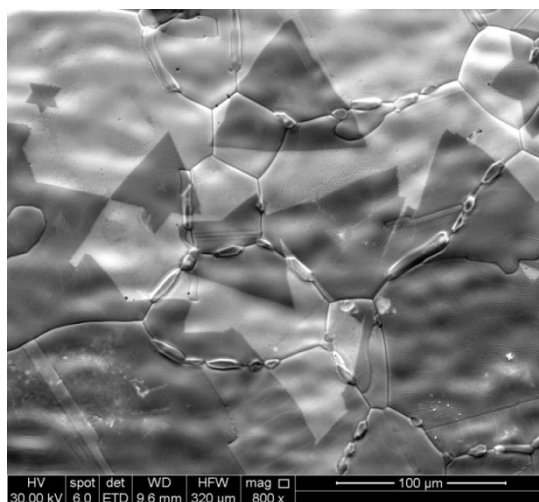


Fig. 3 50-100 nm size single-crystal h-BN triangular domains on Ni

Ismach A., Chou H. et al, in preparation

Dr. Terrones from Penn State University also presented their recent developments on no band gap N-doped graphene (NG) synthesis and its application on molecular sensor.



Results shown monolayer or few layered N-doped graphene can be controlled and synthesized via atmospheric pressure CVD (AP-CVD) process and then transferred to Si/SiO<sub>2</sub> substrate for making device like molecular sensors. Regarding to other layered materials, Dr. Terronesgroup also reported their synthesis and characterization on Tungsten and Molybdenum Disulfide materials. They prepared Molybdenum disulfide (MoS<sub>2</sub>) monolayer on SiO<sub>2</sub> substrates by sulfurization on Mo samples, while Tungsten disulfide (WS<sub>2</sub>) islands materials were prepared by using H<sub>2</sub>S gas and Tungsten oxide thin films at 950C. Both AFM and FEG-SEM showed the triangular cluster formation of WS<sub>2</sub> on substrate, and the most recent results of Raman and photoluminescence (PL) mapping indicated an edge-enhanced photoluminescence property on this specific WS<sub>2</sub> layered material. This edge-enhancement for WS<sub>2</sub> and controlled growth of few layered WS<sub>2</sub> film would be really useful for further application such as photocurrent conducting and electronic devices application.

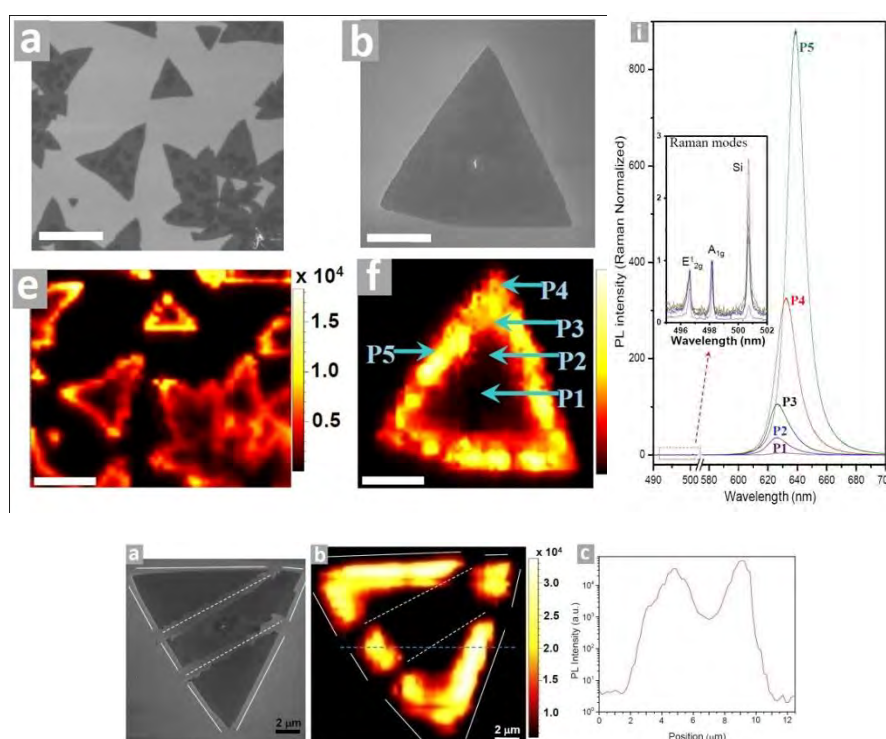


Fig. 4 2D WS<sub>2</sub> islands and edge-enhanced photoluminescence with FEG-SEM images and PL mapping.

*H. R. Gutierrez, N. Perea, H. Terrones, B. Wang, A. L. Elias, R. Lu , V.H. Crespi & M. Terrones, Nano Letters. 2013*

Not only chemical vapor deposition can prepare mono or few layered 2D materials, solution-based chemical exfoliation related results was demonstrated by Dr. Chhowalla and his group. They used Li intercalation exfoliated single layered MoS<sub>2</sub>

exhibited mixed phase structure and their relation to the material properties. There are 2 different structures forming during exfoliation process, trigonal prismatic (2H) and octahedral geometry (1T) phases. These 2 phases have substantially different crystal symmetry which leads to difference in electronic properties. High resolution scanning TEM (STEM) images have shown the strain and coherent interphase between 1T and 2H structures in exfoliated MoS<sub>2</sub> layer materials. Photoluminescence property was also discovered in exfoliated materials. Annealing after exfoliation could also lead to 1T to 2H phase transformation. Devices like FETs made from Au/1T contacts and 2H as active region, showing cooperation of the 2 structures could be possible. These 2D MoS<sub>2</sub> materials were further used for Hydrogen evolution reaction and found out 1T phase showed great reactivity in H<sub>2</sub> reaction. They also found out the reactivity was mainly affected by the basal plane but not the edge of materials structure.

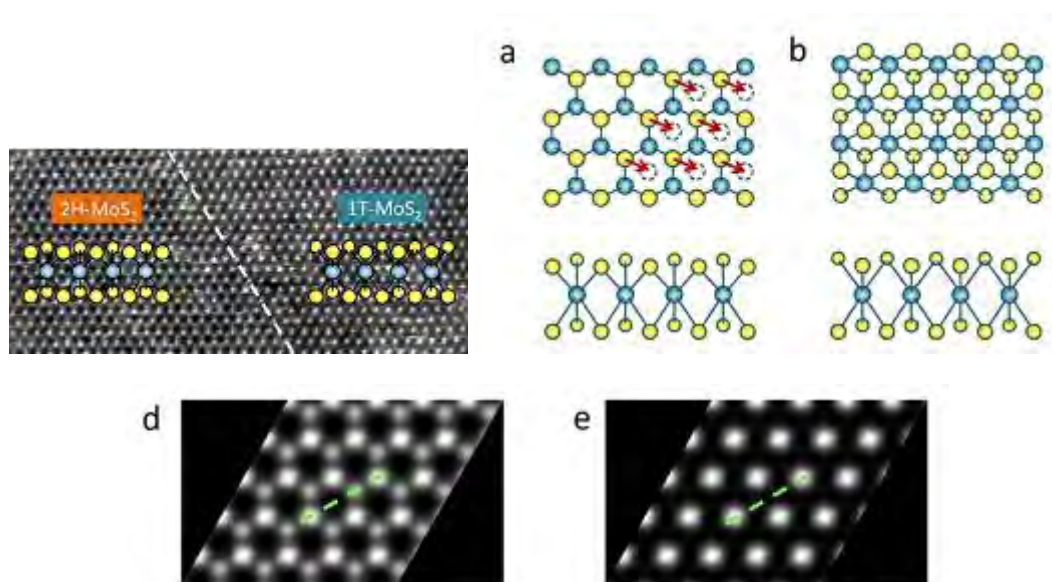


Fig. 5. Mixed phases exfoliated MoS<sub>2</sub> layered thin film and schematic illustration of (a) 2H and (b) 1T crystal structures and their STEM analysis of (d) 2H and (e) 1T. G. Eda, T. Fujita, H. Yamaguchi, D. Voiry, M. Chen, M. Chhowalla, *ACS Nano*, vol. 6, No. 8, 7311-7317, 2012

### PART 3. Theory of 2D Materials

This session in the workshop provided us more information about 2D layered materials from a different point of view – theoretical modeling. Dr. Shenoy from University of Pennsylvania started this session by their recent finding on 1<sup>st</sup> principle calculation modeling 2D materials with heterostructures. He pointed out the 3D stacking and lateral heterostructures can induce interfacial strain that degrade or



damage system. They introduced interfacial stresses from DFT calculation around  $\pm 5$ -20 eV/nm and studied effect of strain on electronic properties on transition metal dichalcogenides and their catalytic activity. From their results, adding  $\sim 1$  eV/nm interfacial stress, lattice mismatch in transitional metal dichalcogenides is only 11% for  $\text{MoS}_2/\text{WTe}_2$  system. Adding tensile strain in transitional metal dichalcogenides systems will decrease kinetic energy, and percentage indirect band gap will increase.

Other important features of single layered metal disulfides  $\text{MS}_2$  ( $\text{M} = \text{W}$  or  $\text{Mo}$ ) such as dislocations, defects and grain boundaries were also be investigated by first-principles calculation. Dr. Yakobson from Rice University predicted the structures of dislocations and assemblies into grain boundaries in 2D metal disulfides materials and h-BN. They found the in-plane and through-layer relaxation results in dislocation cores and concentration of elements at grain boundaries can change the chemical potential of edge and further affect structures. They calculated energy of mixed arm-chair and zig-zag edges through triangular geometry. Their finding on h-BN grain boundaries is related to B-B and N-N pairs (4/8 dislocation) that can change electronic structure. Chemical potential will changes in BN and transitional metal dichalcogenides based on concentration of elements on edge, for example B or N in BN system.

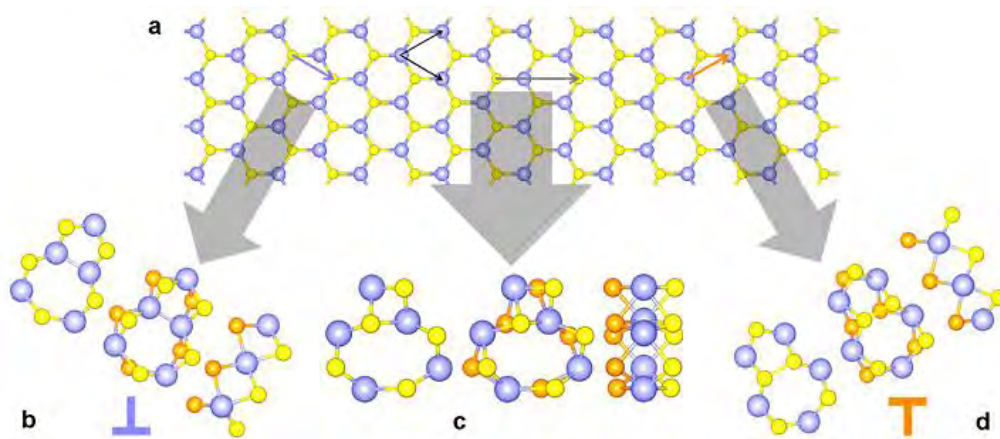


Fig. 6 Basic edge dislocations for 2D metal disulfides.

*X. Zou, Y. Liu, B. I. Yakobson, Nano Letters, No. 13, 253-258, 2013*

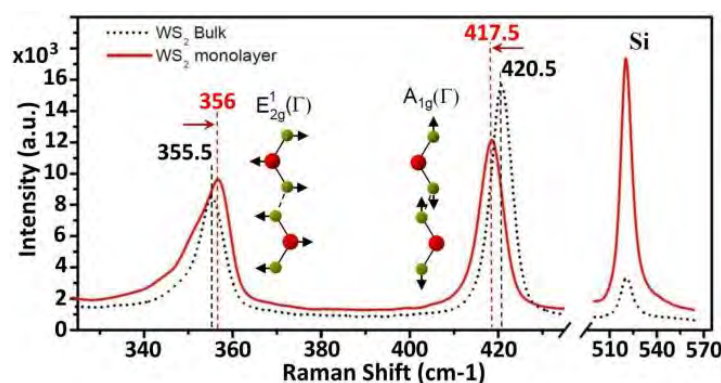
Theoretical calculation on structures of 2D materials plays an important role for understanding them, their piezoelectric properties were also essential for future application. Dr. Reed from Stanford University used density-functional theory calculation probing the piezoelectric coefficients of various monolayer 2D materials including h-BN,  $\text{MoS}_2$ ,  $\text{MoSe}_2$ ,  $\text{MoTe}_2$ ,  $\text{WS}_2$ ,  $\text{WSe}_2$ , and  $\text{WTe}_2$ . Piezoelectric requires insulated bandgap and lack of symmetry, which leads to studies of h-BN with no inversion symmetry and large insulated bandgap. Piezoelectric coefficient of h-BN was

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found to be up to 300pm/V, contrast to the highest of about 9pm/V for MoTe<sub>2</sub> among all transitional metal dichalcogenides materials. They also found out that doping a single sheet of graphene with atoms on one side can break up the inversion symmetry and resulted in piezoelectric graphene materials. Piezoelectric effect does not work for bulk material, Dr. Reed suggested that monolayer stretching and curvature of bilayer, and use of absorbed atoms such as hydrogen or fluoride on graphene materials can be used to induce piezoelectricity.

### PART 4. Properties of 2D Materials

This session focused on the advanced characterization methods for 2D layered materials properties. Dr. Gutiérrez discussed about his exciting findings about WS<sub>2</sub> single and bilayer films and their Raman mapping as well as photoluminescence (PL) investigations. Raman and PL responded as a function of number of S-W-S layers, the increase of S-W-S layers resulted in PL decrease due to change to indirect bandgap in multiple layers. Raman scattering from single to few layered WS<sub>2</sub> was showed excitation laser wavelength in visible range with A<sub>1g</sub> phonon mode decrease and E<sub>2g</sub><sup>1</sup> frequency increase as layered up.



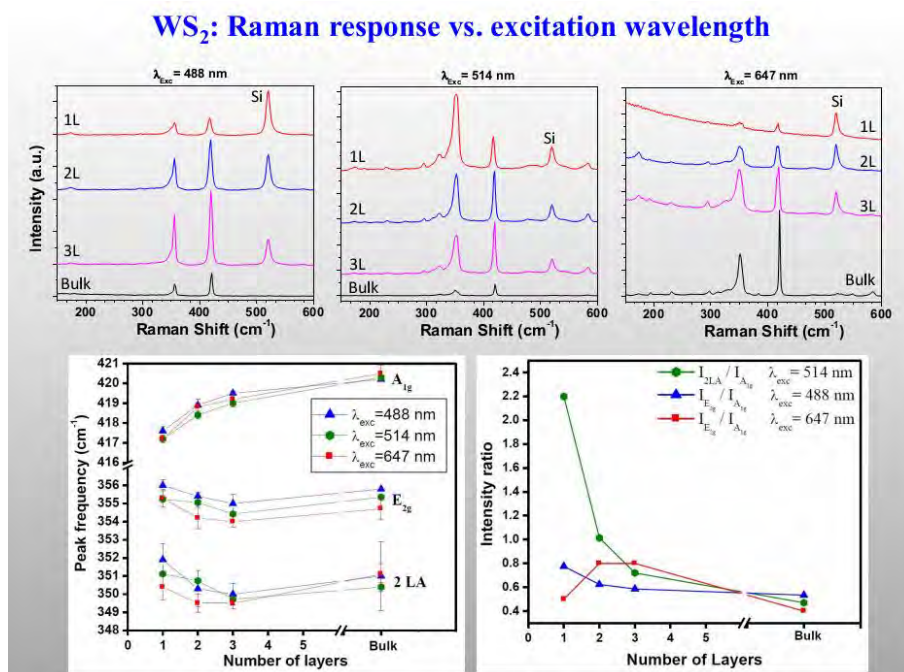
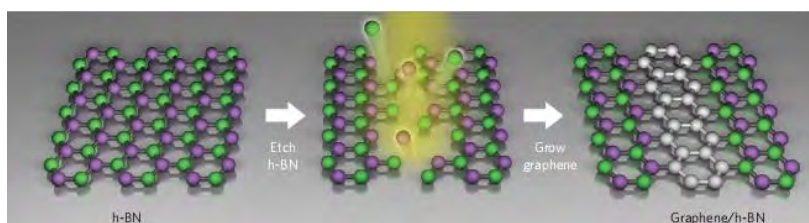


Fig. 7 WS<sub>2</sub> Raman spectroscopy and excitation wavelength.

*H. R. Gutiérrez et al, Nano Letters, ASAP*

Dr. Ajayan from Rice University introduced their work synthesizing and characterizing 2D layered materials and beyond, controlled B-N-C ternary phases for bandgap engineering and growth of graphene in middle of h-BN layered material. According to their research on B-N-C ternary phase diagram, c-BN is stable at low temperature and gains defects after few layers growth. They also reported the property of h-BN protecting Ni from oxidation up to 1100C; it is more difficult to grow graphene on BN compared to BN CVD growth on graphene. Their further studies could focus on mixed layered transitional metal dechalcogenides preparation.



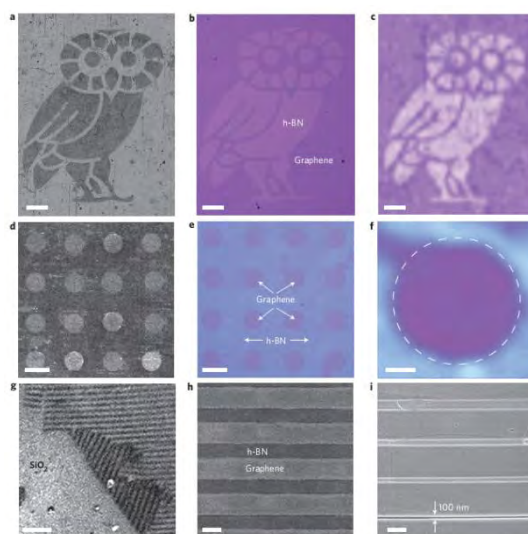


Fig. 8 Creation of micro to nanoscale patterned graphene and h-BN in-plane heterostructure thin film.

*Z. Liu, L. Ma, W. Zhou, Y. Gong, S. Lei, X. Yang, J. Zhang, J. Yu, K. P. Hackenberg, A. Babakhani, J. Idrobo, R. Vajtai, J. Lou, P. M. Ajayan, Nature Nanotechnology, vol. 8, 119-124, 2013*

## PART 5. Devices and Application

Although improvement on preparation methods along with many distinct properties of graphene and other 2D layered materials beyond were discovered, the application for 2D layered materials are still waiting for further development. In this session, a wide variety of applications and devices for 2D layered materials were presented. Dr. Friedman from US Naval Research Lab provided his recent research on chemical vapor sensing by monolayer  $\text{MoS}_2$ .  $\text{MoS}_2$  was chosen among all different transition metal dichalcogenides because its potential for transistor application. It is suitable for chemical sensing with the advantages of a bandgap with good on/off current ratio, and a chemically reactive surface which is important for functionalization.  $\text{MoS}_2$  was investigated for chemical vapor sensors to various analytes and had comparable quality compared to carbon nanotube or graphene sensors. On the other hand, Dr. Shan from Case Western Reserve University demonstrated the possibility for  $\text{MoS}_2$  from a bulk indirect band gap to a direct bandgap atomically thin semiconductor. Atomic structure of  $\text{MoS}_2$  consists of hexagonal planes of S and Mo atoms forming a trigonal prismatic structure that similar to graphene honeycomb but different in having A and B sublattices of either a pair of Mo or S atoms. Different symmetry was the reason for a significant band gap at K/K' point of the Brillouin zone. By optical properties characterization, Dr. Shan showed their finding of quantum confinement

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effect led to indirect gap semiconductor for bulk and direct band gap for monolayer MoS<sub>2</sub> material. They also observed of negative trions, quasi-particles of two electron and hole for monolayer MoS<sub>2</sub> semiconductor interaction, and the possible application on valley and spin-based physics due to its optical helicity.

Dr. Xia from IBM Research Center gave us their point of view for graphene used in photonic device like photodetectors, optical modulators, and linear polarizers based on light-graphene interaction and plasmons in light excitation. They also pointed out using multilayers up to 300nm could lead to better contact for MoS<sub>2</sub> field-effect transistors (FET), while Dr. Appenzeller from Purdue provided another way of solving contact problem is using Sc metal contact. Dr. Appenzeller from Purdue University emphasized the benefit for using two-dimensional materials as FET is thickness controlling aggressive channel length scaling ( $L_{ch} < 3.5\text{nm}$ ). Solving the contact resistance problem, Sc is the best choice for n-type contacts to MoS<sub>2</sub> due to work function match. Mobility of MoS<sub>2</sub> material depends on contact type. According to their observation, MoS<sub>2</sub> with Sc contacts and Al<sub>2</sub>O<sub>3</sub> gate dielectric results in extrinsic mobilities of 700cm<sup>2</sup>/V-s. He also suggested the cooperation of different 2D materials and be using MoS<sub>2</sub> for conduction in charge of electron injection, combined with other 2D materials with good hole injection as a valence band of the transistors.

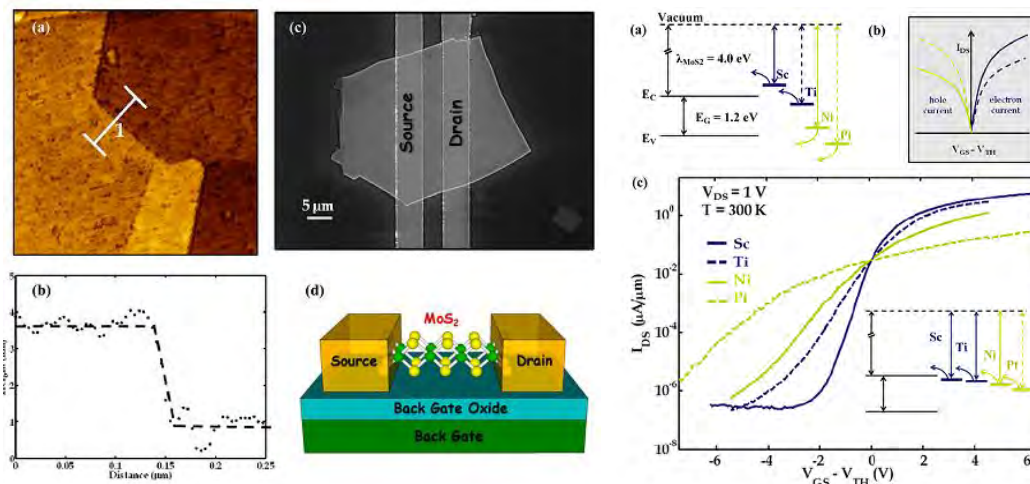


Fig. 9 AFM, SEM, 3D schematic plot and various metal contact materials explaining transfer characteristics of a prototype back-gated MoS<sub>2</sub> transistor.

*S. Das, H.-Y. Chen, A. V. Penumatcha, and J. Appenzeller, Nano Letters, vol. 13, 100-105, 2013*

Dr. Jena from University of Notre Dame started from knowledge we have right now for 2D materials of their chemical bonding, no dangling bonds at interphase, no strain as in 3D heteroepitaxial materials. Base on the measured bandgap of 2D



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materials, Dr. Jena talked about his view of electronic application roadmap. 2D materials are thin and can offer unique advantages with modulation or chemical doping and modify bandstructure symmetry for tunneling Field-Effect transistors (TFET). Stacking of 2D materials can be used for interlayer TFETs and SymFETs with solutions of layers alignment and device processing. DFT bandgap change calculation of and ultrathin BN dielectric can also be used for tunable DOS FETs beyond capacitive control. Dr. Jena also demonstrated their FETs using 10nm wide graphene nanoribbon (Fig. 11), TFETs based on transition metal dichalcogenides such as MoS<sub>2</sub> synthesized by ALD method, and first WS<sub>2</sub> FETs. The on/off ratio of MoS<sub>2</sub> TFT can reach to 10<sup>7</sup> showing good current saturation, and synthesized multilayered MoS<sub>2</sub> can achieve similar performance as exfoliated FETs. Multilayered WS<sub>2</sub> chemically synthesized was made FETs and found still have Schottky contact on the contact. Ga<sub>2</sub>O<sub>3</sub> was used for high voltage large area transistors that could enhance carrier mobility by dielectric engineering.

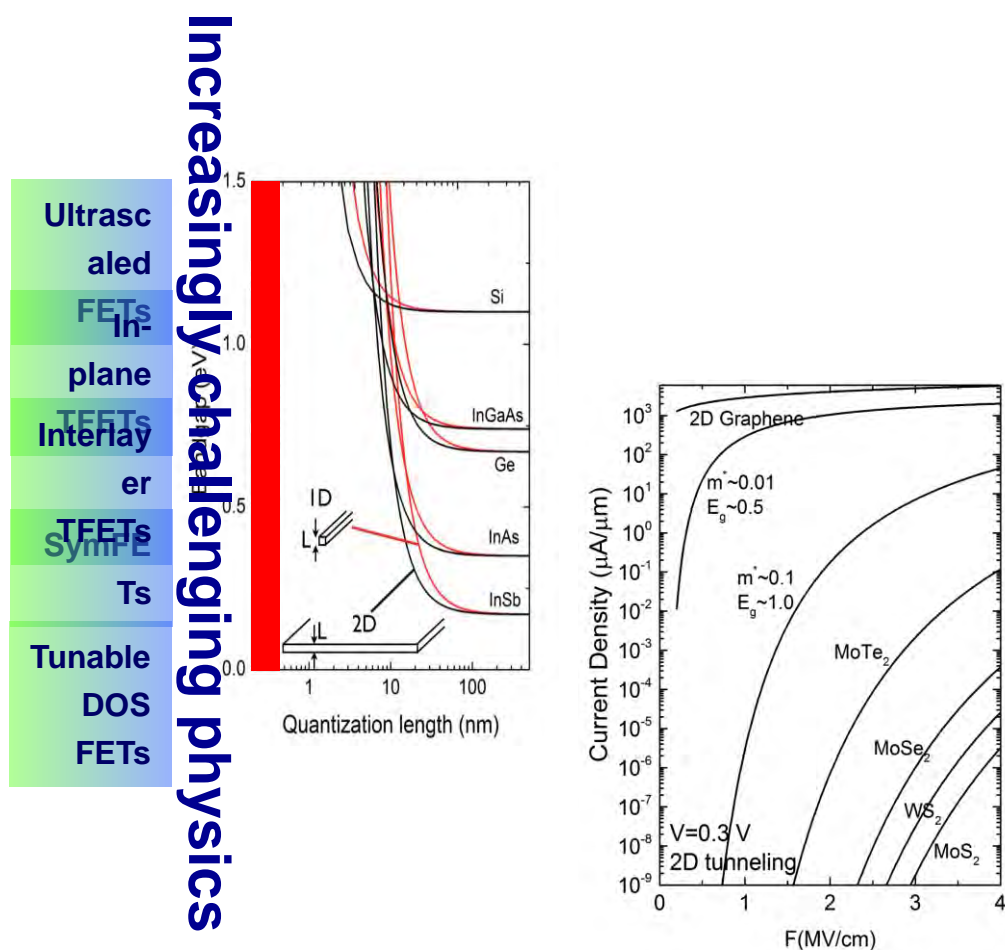


Fig. 10 2D crystal application roadmap from Dr. Jena's presentation.

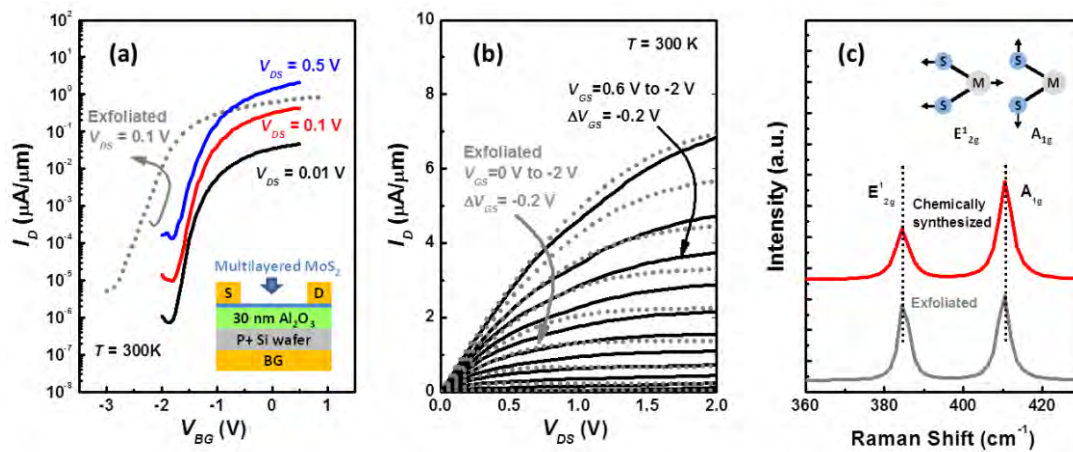


Fig. 12 FETs made and tested for exfoliated and synthesized MoS<sub>2</sub>.

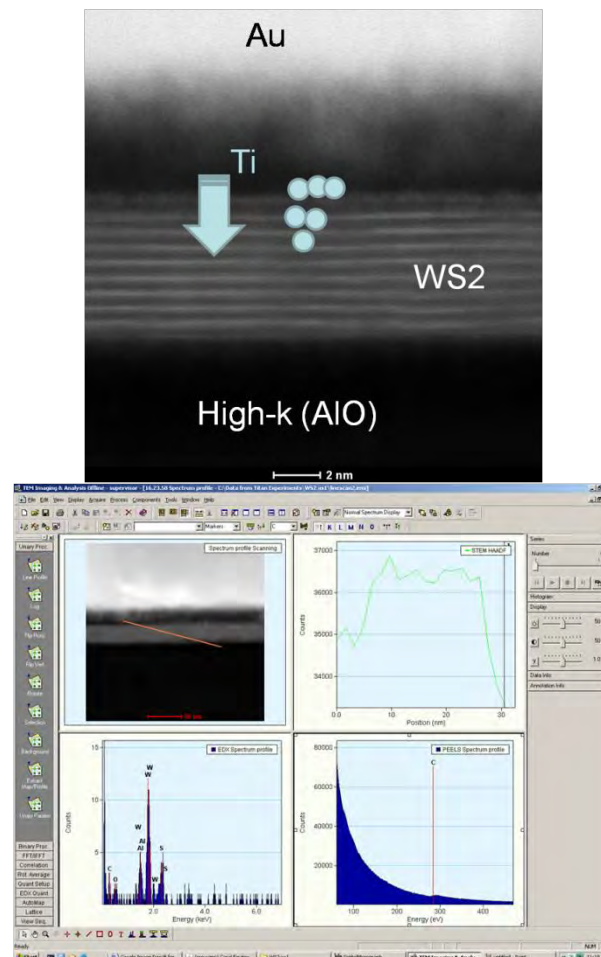


Fig. 13 EELS measurements on WS<sub>2</sub> FETs demonstrated Schottky effect for Ti is diffused into WS<sub>2</sub>(spot size 0.2~0.3nm)

*Dr. Jena's presentation in Beyond Graphene Workshop*

Dr. Salahuddin from Berkeley also discussed that although MoS<sub>2</sub> transistors have

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high on/off ratio, the lack of degeneracy, low mobility with increase of thickness still need improvement. MoS<sub>2</sub> transistors could be a good fit for mid-range saving device rather than high performance devices. Results of MoS<sub>2</sub> with a-Si for photodetector showed 10x improvement in photocurrent compared to a-Si photodetector. They also suggested 2D heterostructure could be a new solution for high performance transistors due to free dangling bonds and defects from Van der Waal interface between layers.



## **V. Beyond Graphene Panel Discussion Digest: Now and Future**

### **Discussion Overview**

In the device (and materials) community there is an ever-increasing push for speed, power, and sensitivity. To meet this challenge, advances in materials and devices have led to novel materials and devices. The discovery graphene and other semiconducting 2D crystals have led to an explosion of device R&D that utilize low dimensional material systems to achieve the above challenges. These breakthroughs have opened up the possibility of exploring the fascinating properties of novel devices.

But scientists and engineers have made claims that each are the ideal candidate in multiple applications. In spite of excellent progress in nanofabrication techniques during the last decade, the scientific community has yet to reach a consensus the full potential of graphene and other 2D Materials, leading to the questions:

- **Where can the low dimensional material systems out-perform their “3D” counterparts?**
- **What device architectures may best take advantage of the unique properties of 2D layered materials to truly provide a path to superior performance in DoD applications?**

Answering these questions and more were the focus of the panel session.

### **1. Searching for certain applications that can make 2D materials valuable**

<b>Current Development Status</b>	<b>Looking forward</b>
<ul style="list-style-type: none"><li>➤ Difficult to find a certain electronic device to use 2D materials.</li><li>➤ Many trade-offs need to consider thoroughly pursuing high performance devices.</li><li>➤ 2D materials could be really useful due to very large band gap and higher on/off ratios than other materials cannot.</li><li>➤ Unless there is a brand new</li></ul>	<ul style="list-style-type: none"><li>➤ Probing new applications as we move on understanding the features.</li><li>➤ More input in searching applications should be done quickly.</li><li>➤ We should not use hole mobility to judge the potential of 2D materials.</li><li>➤ Low power electronic device could be the way out for high on/off ratio with a low leakage current.</li><li>➤ We should always keep in mind that</li></ul>

<p>application that cannot be exist without 2D materials, it will still be really hard to justify that it's a good materials for future or not.</p>	<p>other techniques, including silicon technologies are all getting better as we move on.</p> <ul style="list-style-type: none"> <li>➤ Need to use the biggest advantage of these 2D materials – for sub-nanometer regime.</li> <li>➤ Large band gap of 2D material does not mean we cannot get good contact in transistors, but seek other application that can use this feature.</li> <li>➤ Doping 2D materials could possibly solve the essential contact problems for making transistors.</li> <li>➤ Need to explore more in tunneling properties see if we can open new applications that only for 2D materials.</li> </ul>
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## **2. Heterostructures of beyond graphene 2D materials**

- Heterojunctions between layers will affect the performance due to Van der Waals bonding layered but not for 2D materials.
- Heterojunctions of 2D materials could yield direct access to spin, not possible in 3D semiconductors.
- Need to understand the exact bandgap for monolayer 2D materials thoroughly.
- Need to improve or change the fundamental knowledge so we can actually evaluate vertical tunneling conduction band, but not using previous experience based on nanotubes.
- Building basic database for 2D materials especially transitional dichalcogenides and more will be beneficial for understanding the full range of conduction bands and the theory.
- Heterostructures and their application on photodetection can give 10 times faster response than a-Si diodes, still need to be improved on this direction.

## **3. Approach of optical applications for 2D materials**

- 2D materials indeed have extraordinary performance in quick response. Some transitional dichalcogenides like MoS<sub>2</sub> monolayers have valley polarization that other materials didn't have at all.

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- The band gap is about 1-2eV for 2D materials, close to visible light region that can be used for light directing chip.
- Need to find out more about photodetectors application that can be used in photoemitters and investigate their efficiency.
- Easily stacking for 2D materials can also benefit photodetector development in cooperating III-V photoemitters. 2D and III-V materials cooperation could let us understand more about 2D materials in this application.
- Solving the inject holes contact problem would be essential for moving forward in optical application.

**4. Piezoelectric Feature of 2D materials**

- For theoretical point of view, these materials are really interesting probing their piezoelectric and some other properties.
- Started from graphene, and all other similar layered structure materials, and their stacking-up, we need to figure out what's the structure of these materials, how do they stack, are all important information to help us address the issue of basic properties in this field.
- Need to have more input on characterization of these 2D materials for probing in piezoelectric application.

Funding Acknowledgements



**Beyond Graphene Workshop Survey: Improving for Next Year**

**Registration:**

- How did you register? Online \_\_ (13) \_\_ Mail \_\_\_\_\_ Fax \_\_\_\_\_  
Phone \_\_\_\_\_
- Registration Process 1 \_\_\_\_\_ 2 \_\_\_\_\_ 3 \_\_\_\_\_ 4 \_\_ (1) \_\_ 5  
\_\_\_\_ (12) \_\_ N/A \_\_\_\_\_
- Suggestions for improvement
  1. Provide info on the ways of payments before initiating the registration process
  2. Sources of internet not provided
  3. No free internet access available for attendees. Hope internet access can be available freely for attendees
  4. Email was forwarded to me about the event

**Marketing:**

- Marketing informative - timely (i.e., date saver cards, e-mail alerts) 1  
\_\_\_\_\_ 2 \_\_ (3) \_\_ 3 \_\_ (4) \_\_ 4 \_\_ (5) \_\_ 5 \_\_ (4) \_\_
- Suggestions for improvement
  1. Workshop location not clarified
  2. Late advertising

**Talks:**

**Synthesis Presentations**

- Relevance 1 \_\_\_\_\_ 2 \_\_\_\_\_ 3 \_\_\_\_\_ 4 \_\_ (6) \_\_ 5 \_\_ (10) \_\_
- Quality 1 \_\_\_\_\_ 2 \_\_\_\_\_ 3 \_\_\_\_\_ 4 \_\_ (7) \_\_ 5 \_\_ (7) \_\_
  1. Too much information. Too many slides. Talks were not organized for a half hour crisp presentation
  2. All the talks are really great and discussion with committee members

**Theory Presentations**

- Relevance 1 \_\_\_\_\_ 2 \_\_\_\_\_ 3 \_\_\_\_\_ 4 \_\_ (7) \_\_ 5 \_\_ (9) \_\_
- Quality 1 \_\_\_\_\_ 2 \_\_\_\_\_ 3 \_\_\_\_\_ 4 \_\_ (6) \_\_ 5 \_\_ (7) \_\_
- Suggestions for improvement
  1. First talk (Shenoy) very good. Second talk (BIY) really bad. Third talk ok. For the last two, too many slides – not prepared for a half an hour presentation

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2. It would be good if it increases the #of talks

**Device Presentations**

- Relevance 1 \_\_\_\_ 2 \_\_\_\_ 3 \_\_\_\_ 4\_(6)\_\_\_\_ 5\_(9)\_\_\_\_
- Quality 1 \_\_\_\_ 2 \_\_\_\_ 3 \_\_\_\_ 4\_(7)\_\_\_\_ 5\_(8)\_\_\_\_
- Suggestions for improvement

**Properties/Characterization Presentations:**

- Relevance 1 \_\_\_\_ 2 \_\_\_\_ 3 \_\_\_\_ 4\_(8)\_\_\_\_ 5\_(9)\_\_\_\_
- Quality 1 \_\_\_\_ 2 \_\_\_\_ 3 \_\_\_\_ 4\_(7)\_\_\_\_ 5\_(5)\_\_\_\_
- Suggestions for improvement
  1. Too many slides. Not a crisp informative talk
  2. Order of presentation can be optimized e.g., have the basic characterization on the first day

**Panel Discussion:**

- Relevance 1 \_\_\_\_ 2\_(2)\_\_\_\_ 3\_(2)\_\_\_\_ 4\_(1)\_\_\_\_ 5\_(10)\_\_\_\_
- Quality 1 \_\_\_\_ 2\_(2)\_\_\_\_ 3\_(2)\_\_\_\_ 4\_(3)\_\_\_\_ 5\_(6)\_\_\_\_
- Suggestions for improvement
  1. I missed this
  2. Did not attend

**Other areas of focus you would be interested in?**

1. Device and application in broader range
2. Spintronics, low temp measurements
3. I thought the workshop went well. I enjoyed the length of the presentations and the ability to interact with the other research groups
4. Assembly

**MSC Tour:** 1 \_\_\_\_ 2 \_\_\_\_ 3 \_\_\_\_ 4\_(3)\_\_\_\_ 5\_(2)\_\_\_\_

- Suggestions for improvement
  1. I missed this
  2. Did not attend

**Poster presentations:**

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- Relevance                    1 \_\_\_\_ 2\_(1)\_\_\_\_ 3\_(4)\_\_\_\_ 4\_(3)\_\_\_\_ 5\_(8)\_\_\_\_
- Quality                    1 \_\_\_\_ 2\_\_\_\_ 3\_(5)\_\_\_\_ 4\_(4)\_\_\_\_ 5\_(5)\_\_\_\_
- Suggestions to strengthen our poster session
  1. There was no focus on the poster session, it was almost non-existent
  2. It was not inclusive enough, amount of posters was very low
  3. Did not attend
  4. Poster session was not very engaging (perhaps people were just tired)
  5. I would suggest having more posters or at least a better showing from universities other than Penn State

**Facilities:**

- Conference facilities    1 \_\_\_\_ 2\_\_(3)\_\_\_\_ 3\_(4)\_\_\_\_ 4\_(4)\_\_\_\_ 5\_\_\_\_  
\_(5)\_\_\_\_
- Suggestions
  1. Internet access, parking convenience
  2. Free wi-fi and perhaps a better location for a quick lunch
  3. The projector was very bad, the room was comfortable though
  4. Screen is too small
  5. Better coffee would help – too weak
  6. Projector was finicky; food was sub-par

**What are your thoughts on the overall usefulness of the workshop?**

1. It's a great opportunity to get an overview on the 2D material research going on
2. See other areas of focus
3. Very useful to push the field/boost collaboration. One social event would have been nice. Dinner or lunch. Consider putting together a board for next year (an inclusive one)
4. Pretty useful, and the material was highly relevant
5. Excellent! Great job by organizers!

**What didn't you like about the workshop?**

1. I actually think the panel session could have been longer. It was nice to see professors speak openly about their thoughts on the field.
2. No lunch. Cold food
3. Nothing

**Please provide any suggestions for improvements in the future?**

1. Engage graduate students – how do we fit in the roadmap? How should we be involved in the path forward? We are not experienced

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in making such high-level/big picture decisions. Personally, I would like to learn about the process

**What subjects would you like to see presented in future?**

1. More on heterostructures, more long-term perspective
2. Keep at PSU and keep with MURI review if possible (great venue)